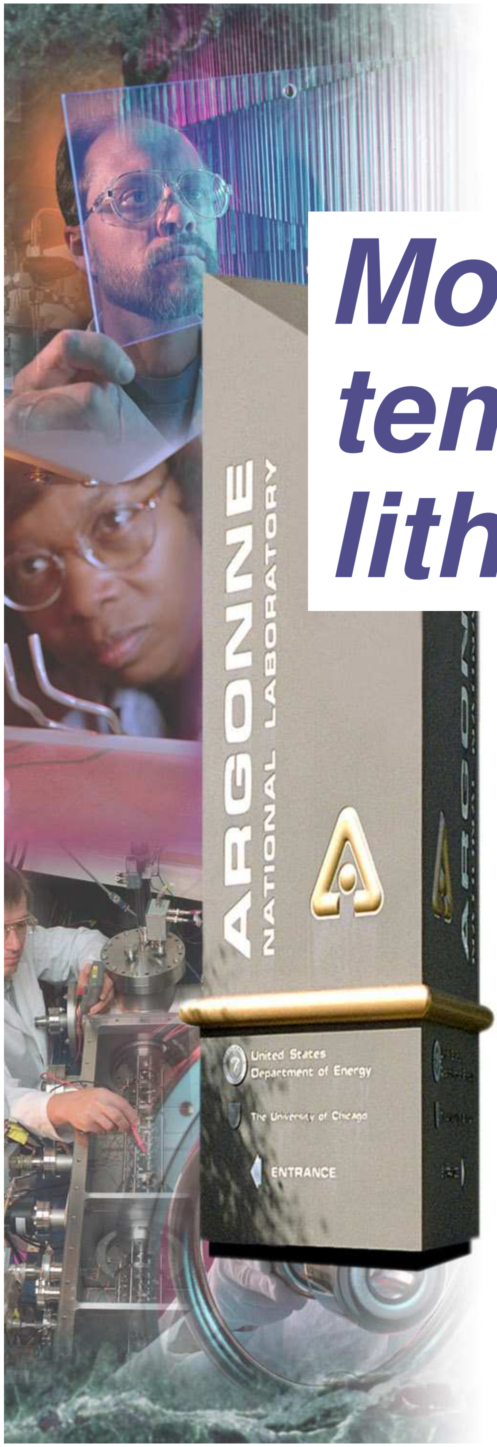

Modeling and analysis of temperature -dependent lithium erosion by plasma

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Outline

- Molecular Dynamics model
- Sputtering solid-liquid Lithium by He+ ions
  - Energy dependence at 10-150 eV
  - Temperature dependence for T=50 -700K
- MD of Li sputtering by He bubble splashing
- Bubble splashing model

Analytical EAM-Li-Li potential

We used the ion-ion potential (1) for Lithium [1]. He-He potential was chosen of a (exp-6) type [2]. Li-He potential was obtained by two ways: the Lorentz-Berthelot rule (#1) and from quantum mechanics (#2) from [3].

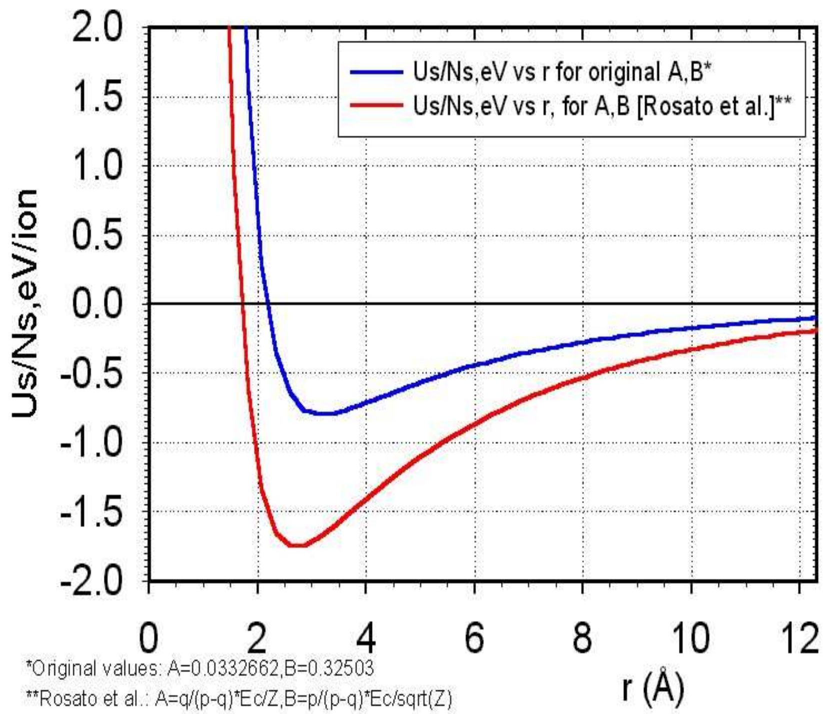
$$U_{coh} = U_{rep} + U_{atr},$$

$$U_{rep} = \sum_i \varepsilon_0 \sum_{j \neq i} \exp\left[-p\left(\frac{r_{ij}}{r_0} - 1\right)\right], \qquad (1)$$

$$U_{atr} = -\sum_i \left\{\sum_{j \neq i} \varsigma^2{}_0 \exp\left[-2q\left(\frac{r_{ij}}{r_0} - 1\right)\right]\right\}^{1/2}$$

Parameters used for this simulation:

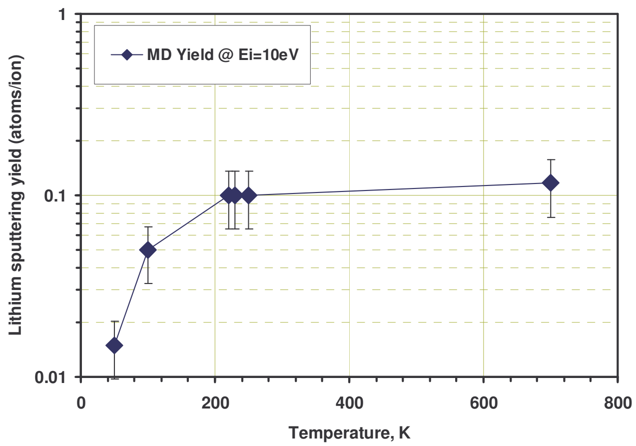
	ε_0, mRy	ς_0, mRy	p	q	r_0, a.u.
Li-Li:	2.4450	23.889	7.75	0.737	5.490
He-He:	0.0694		14.5		5.61
Li-He#1:	1.52		14.5		5.55
Li-He#2:	2.35				3.57

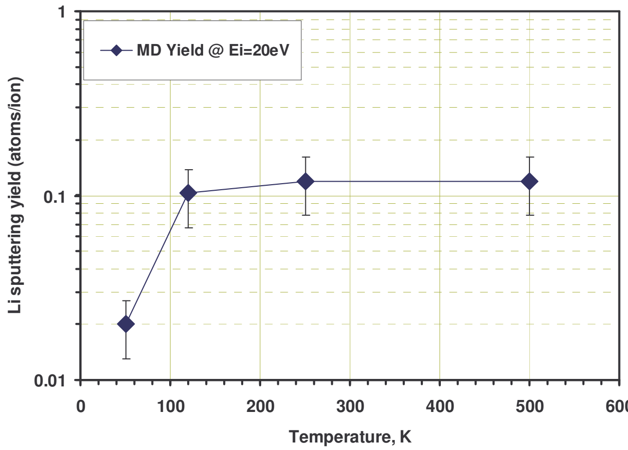


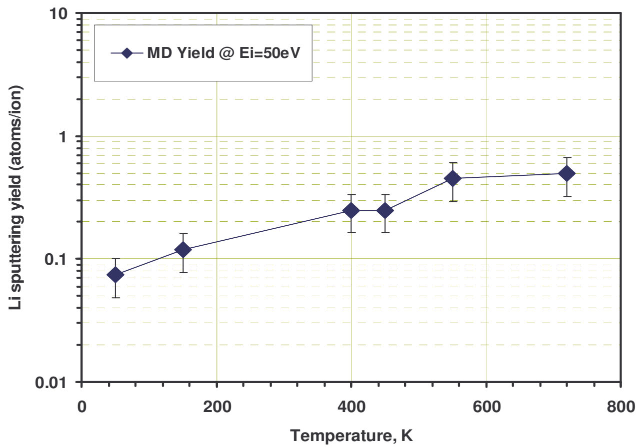
*Original values: A=0.0332662,B=0.32503
**Rosato et al.: A=q/(p-q)*Ec/Z,B=p/(p-q)*Ec/sqrt(Z)

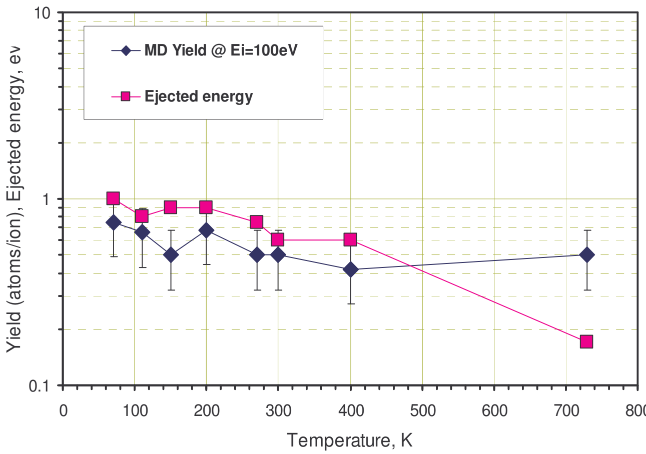
Reference:
[1] Y. Li et al, Phys. Rev. B57 (1998) 15519.
[2] R.A. Aziz et al, JCP 94 (1991) 8047.
[3] P. Soldan, Chem.Rev.Lett. 343 (2001) 429.

Li sputtering Yield vs T,K @10-150eV

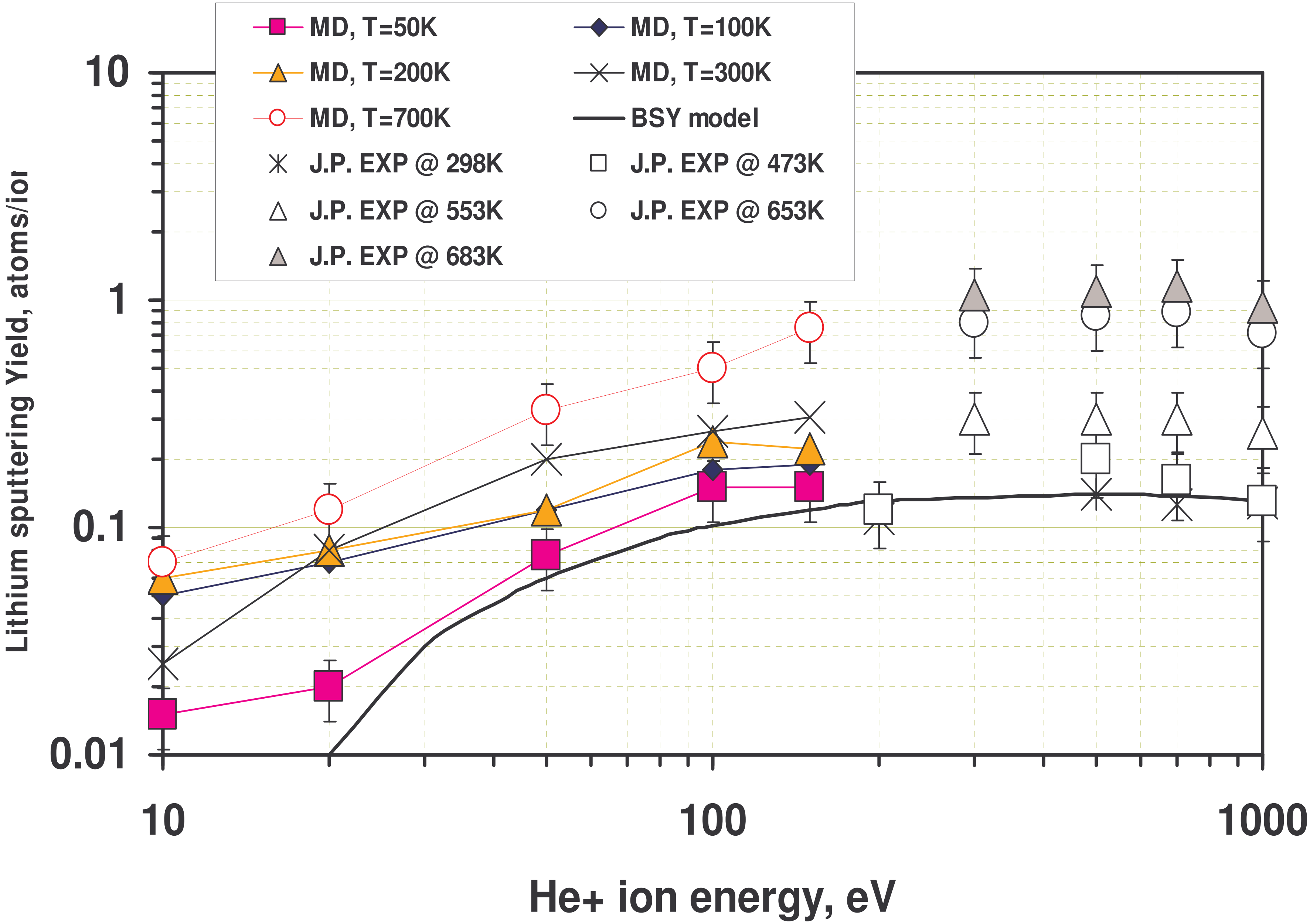








Comparison of MD calculations with experiment



Experiments at different temperatures

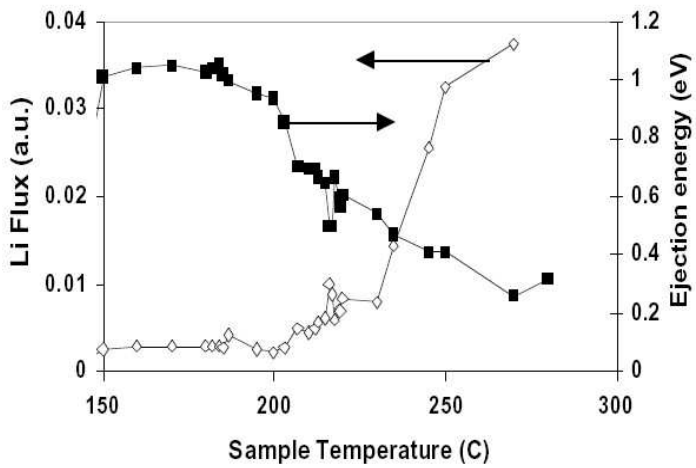


Figure 3. Spectroscopic measurements showing the temperature dependence of the eroded lithium atomic flux from a sample, and the ejection energy of the eroded lithium atoms.

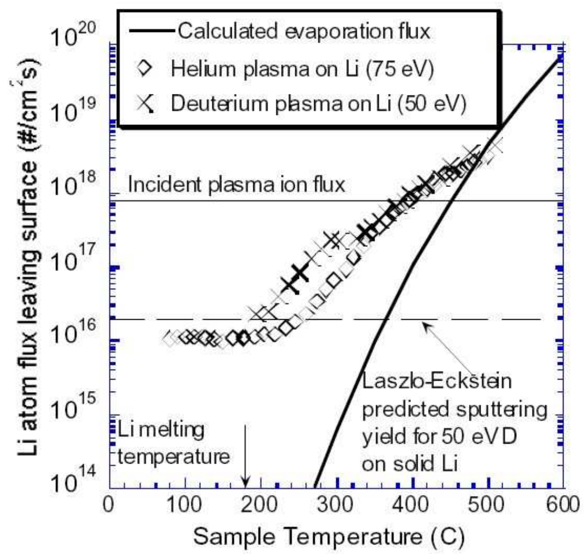
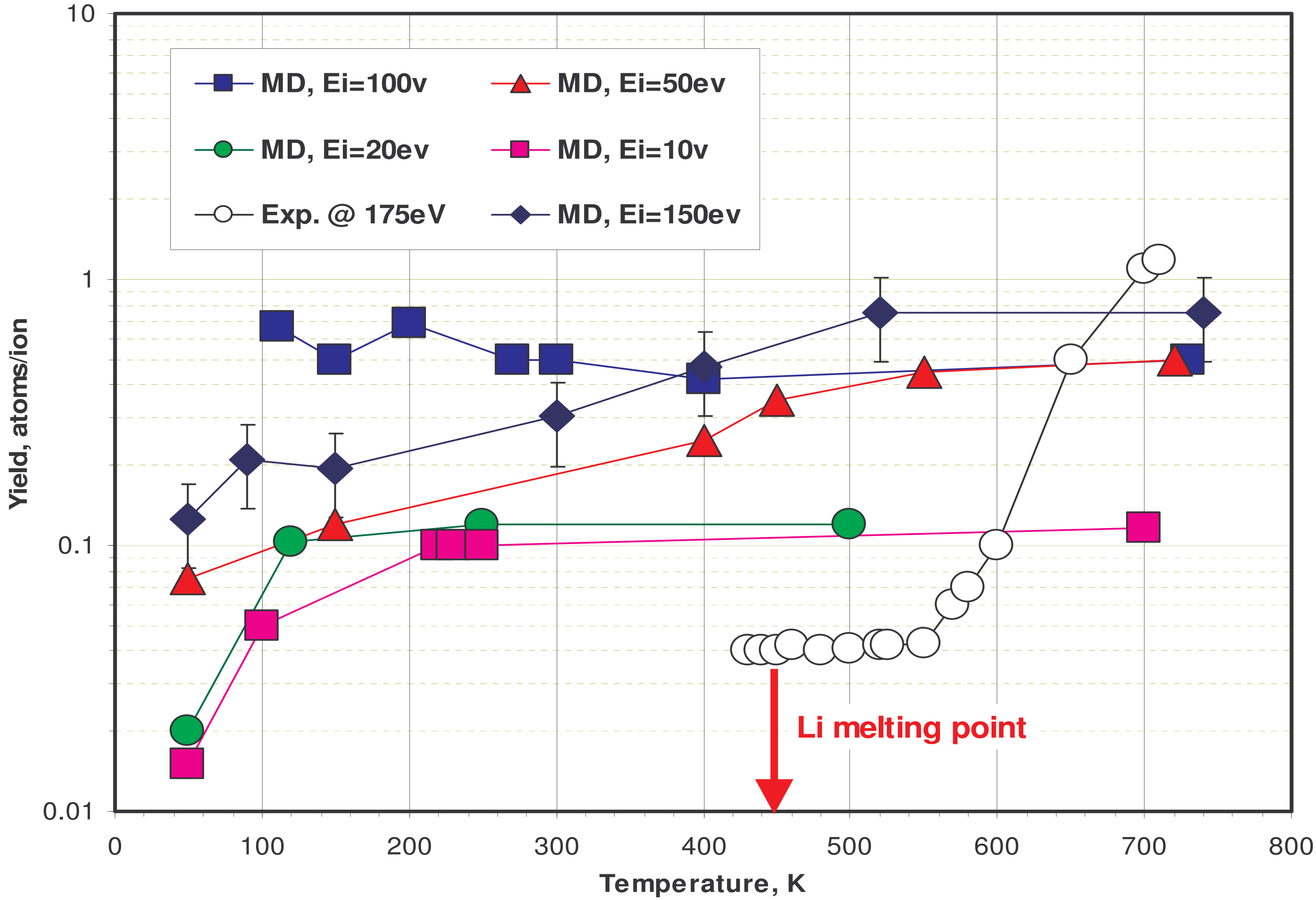


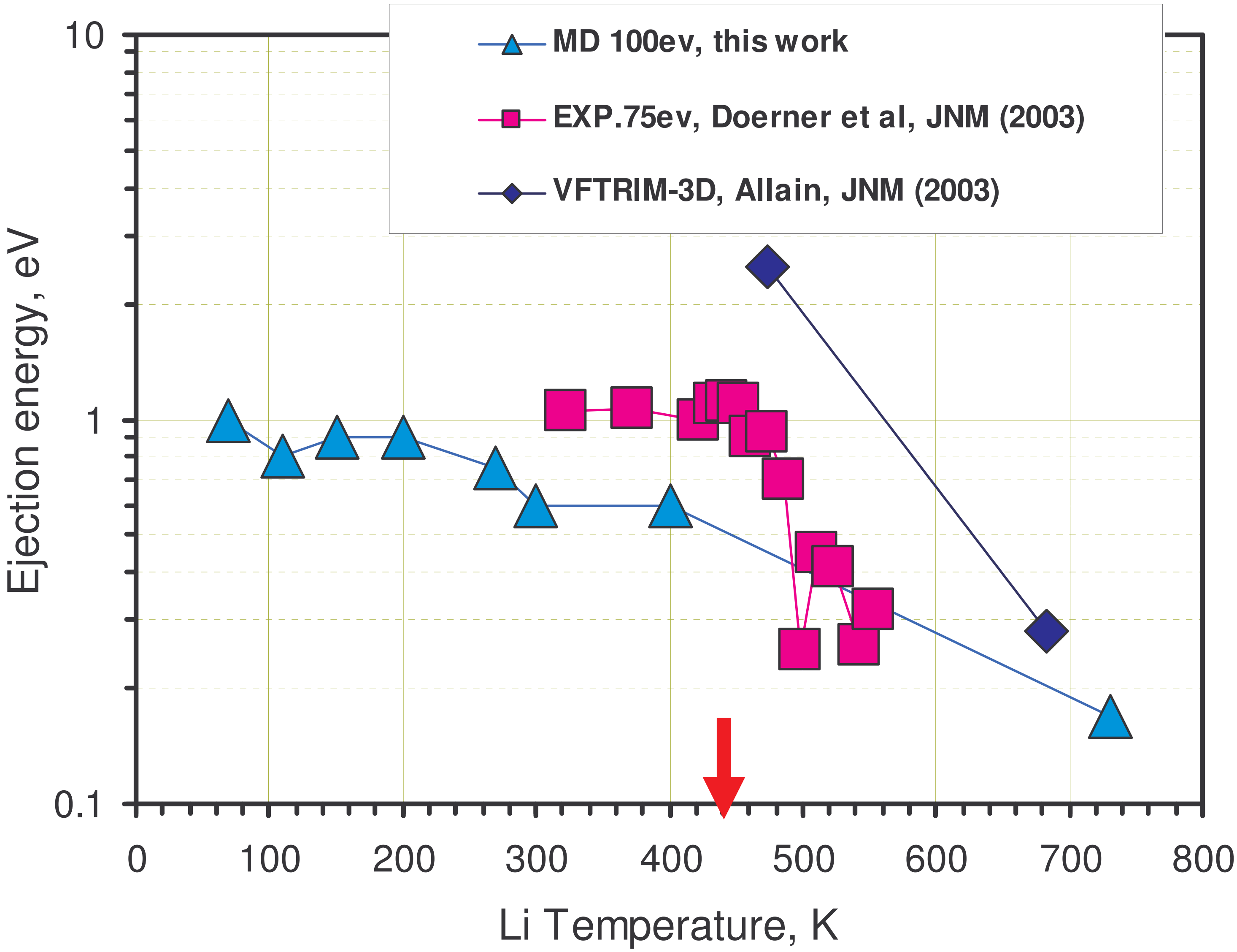
Figure 4. Lithium efflux as a function of temperature in PISCES-B. At low temperature, near the phase transition, the loss rate coincides with that expected from physical sputtering. At high temperature (T>500C) the loss rate converges to the evaporation rate. The loss rate diverges from expectations between these two limits.

Doerner et al, ***Journal of Nuclear Materials***
Volumes 313-316 , March 2003, Pages 383-387

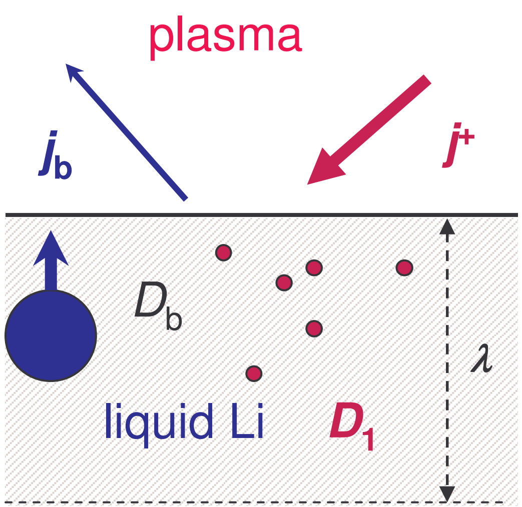
MD yield vs T,K, E - parameter



Li ejected energy: MD vs TRIM, Experiment



He bubble splashing model



$$\gamma = 0.4307 - 1.6262\times 10^{-4}\times T(^\circ C)$$

$$\lambda = 10^{-6}\,m,\ t = 10^3\,s,\ D_1 = 10^{-9}\,m^2 s^{-1}$$

$$Y_b = \alpha j_b / j^+,\quad C_b = C_1 B \exp\left[-\Delta G^* / kT\right] = C_1 B\cdot\varepsilon,$$

$$j_b = n_b^*(t) C_b \bar{v} = \frac{4}{3}\pi R_0^3 \rho_b \exp\left[3\left(\frac{3\beta_D}{4}\cdot\frac{kT}{\gamma}\cdot j^+\cdot t\right)\right]\cdot C_1 B\cdot\varepsilon\cdot\bar{v},$$

$$C_1 = j^+ \frac{\lambda}{D_1}\frac{1}{1+n_b^*(t)\cdot\varepsilon}$$

- **We have calculated ΔG^* for an empty cavity but it is unknown for a cavity filled with Helium.**
- **The parameter β_D is also unknown – need more work;**
- **We also need D_b – the bubble diffusion coefficient**

Low bubble concentration

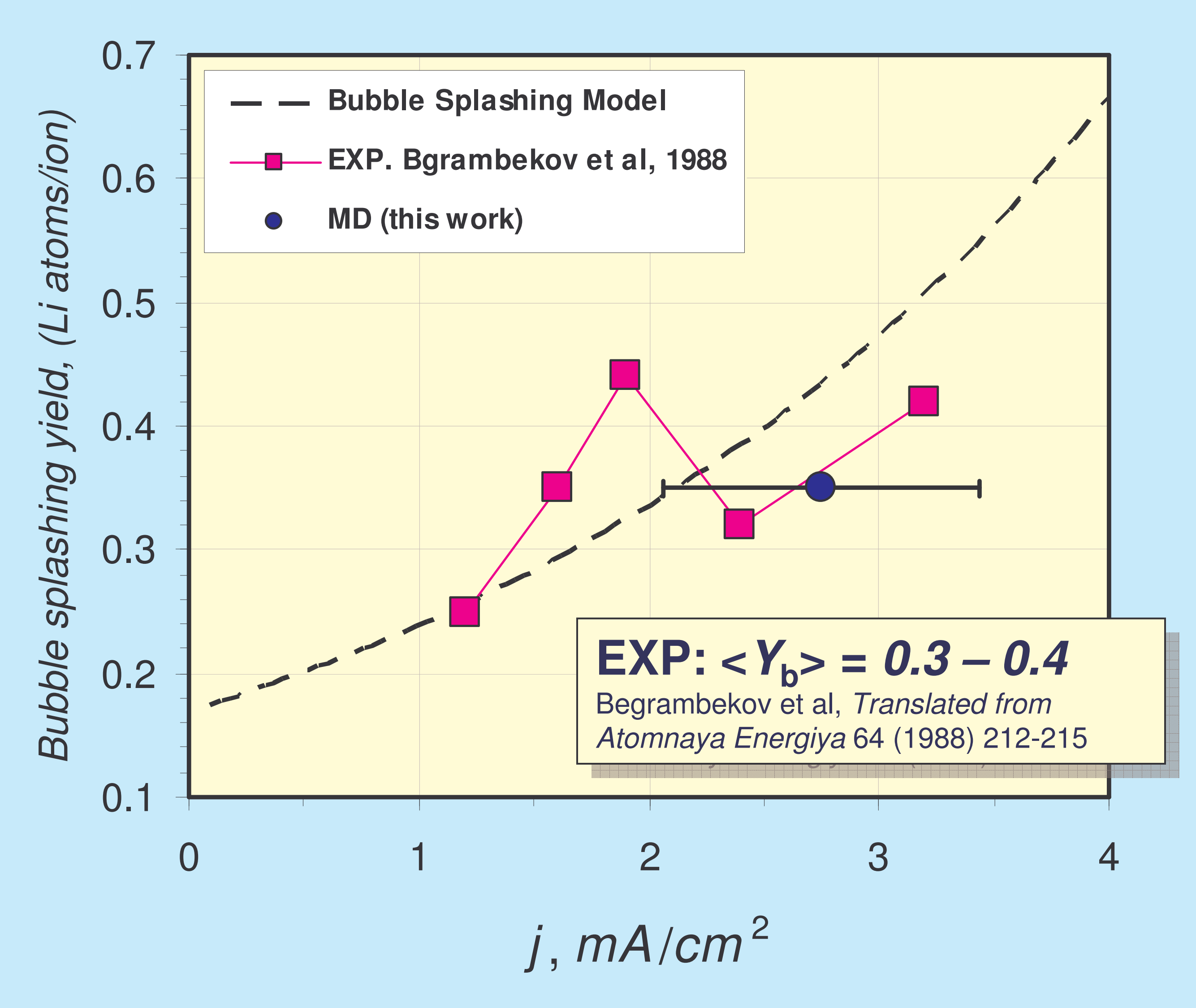
If $n_b^*(t)\cdot\varepsilon << 1,$

$$Y_b = \alpha\,\rho_b\cdot\frac{4}{3}\pi R_0^3 \exp\left[3\left(\frac{3\beta_D}{4}\cdot\frac{kT}{\gamma}\cdot j\cdot t\right)\right]\cdot const$$

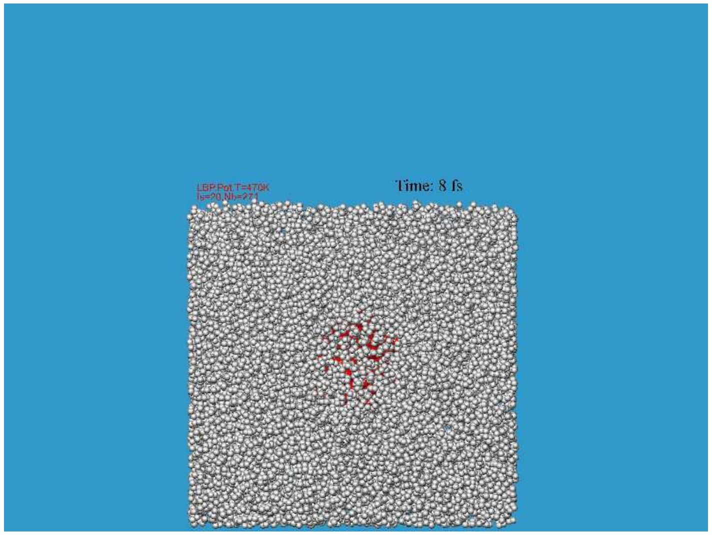
For low fluxes (<1 mA/cm2), the bubble sputtering yield is negligibly small because the concentration of bubbles is small

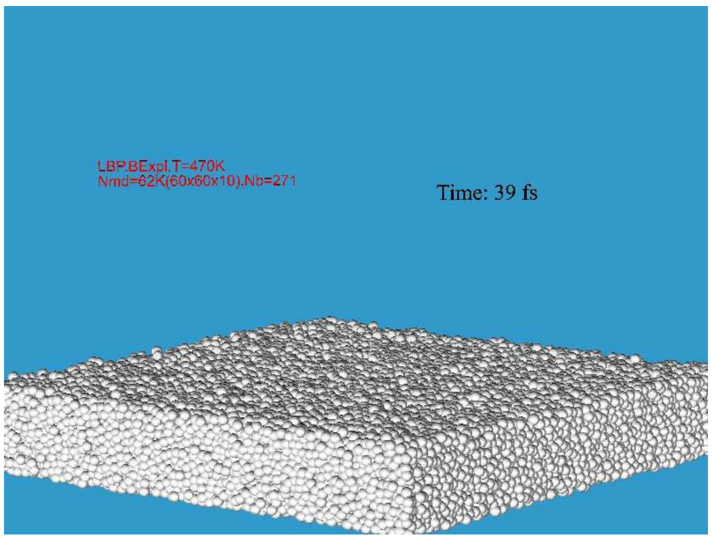
For high ion fluxes, the bubble sputtering yield gives the main contribution to the total yield

Comparison with experiment

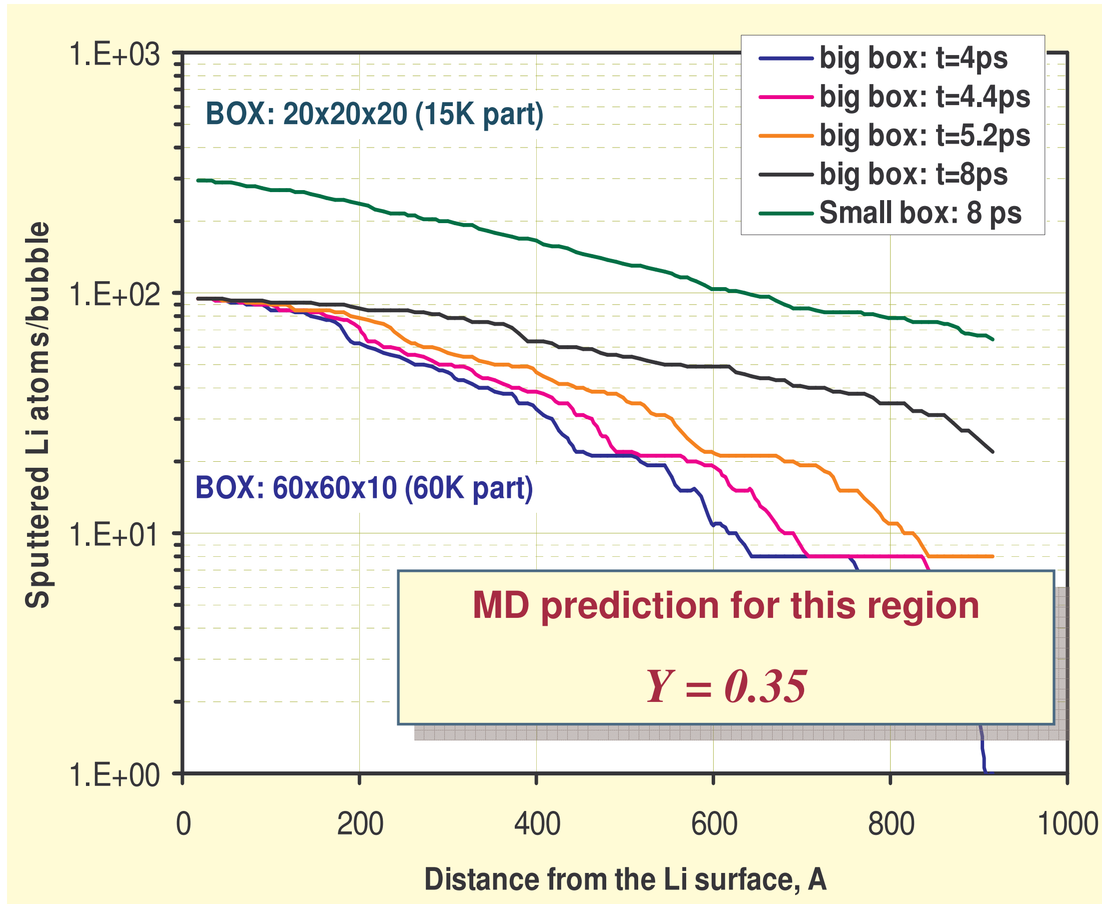


MD of He bubble splashing





Sputtering yield produced by bubble splashing



Summary

- The sputtering yields and energies of Lithium atoms irradiated with He+ ions, with energies of 10-150 eV, were calculated by MD method at various temperatures below and above the melting temperature and compared to experimental data

- A simple model of bubble splashing at low bubble concentrations gives a reasonable yield increase with the ion flux increase. To develop this model any further we will need to do more simulations of bubble formation, the bubble concentrations and the formation energies

- The sputtering yield by the bubble splashing mechanism calculated by MD is in excellent agreement with experiment at higher ion fluxes

- We need more understanding on the "new" <u>premelting effect</u> that we have found in the simulation of the solid Li close to the melting point